Study on the Anticoagulant or Procoagulant Activities of Type II Phenolic Acid Derivatives

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1. Melting points and spectral data

1.1 Caffeic acid derivatives

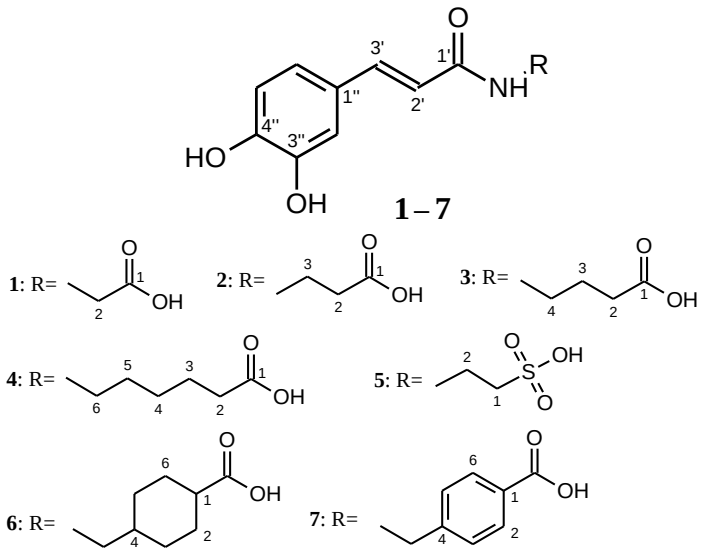


Figure S1 The Structures of Cds. **1–7**

Table S1 ^{13}C NMR Data of Cds. **1–7** (151 MHz, DMSO-d_6)

	Cd. **1**	Cd. **2**	Cd. **3**	Cd. **4**	Cd. **5**	Cd. **6**	Cd. **7**
–COOH	N/A	N/A	N/A	N/A	N/A	176.82	168.29
C-1	172.87	173.43	177.65	174.59	50.71	44.80	131.84
C-2	43.89	34.43	35.13	33.70	35.71	29.56	129.47
C-3	N/A	35.41	25.98	24.34	N/A	28.35	127.13
C-4	N/A	N/A	35.29	26.14	N/A	37.20	143.74
C-5	N/A	N/A	N/A	29.06	N/A	28.35	127.13
C-6	N/A	N/A	N/A	38.58	N/A	29.56	129.47
C-1′	165.12	165.99	165.63	165.41	165.25	165.47	165.80
C-2′	118.87	118.80	118.54	118.67	118.52	118.66	118.10
C-3′	138.98	139.65	139.22	139.01	139.16	139.02	139.90
C-1″	126.38	126.83	125.84	126.51	126.35	126.50	126.32
C-2″	114.25	114.28	114.29	113.88	113.93	113.87	114.25
C-3″	146.10	145.96	145.56	145.59	145.55	145.55	145.86
C-4″	147.94	147.74	148.81	147.67	147.36	147.26	147.82
C-6″	120.38	120.89	120.31	120.44	120.40	120.37	120.63
–CH_2–	N/A	N/A	N/A	N/A	N/A	42.57	42.16

Table S2 ^{1}H NMR Data of Cds. **1**–**7** (600 MHz, DMSO-d_6)

	Cd. **1**	Cd. **2**	Cd. **3**	Cd. **4**	Cd. **5**	Cd. **6**	Cd. **7**
–COOH	N/A	12.15 (1 H, s)	N/A	12.02 (1 H, s)	N/A	N/A	N/A
–OH	N/A	9.28 (2 H, s)	N/A	9.27 (2 H, d)	9.24 (2 H, d)	9.25 (2 H, d)	4.30 (1 H, s, –OH-3″), 4.29(1 H, s, –OH-4″)
–CONH–	7.57 (1 H, t, *J* = 4.80 Hz)	8.07 (1 H, t, *J* = 5.46 Hz)	8.17 (1 H, s)	7.98 (1 H, t, *J* = 5.64 Hz)	7.93 (1 H, t, *J* = 5.55 Hz)	7.95 (1 H, t, *J* = 5.82 Hz)	8.64 (1 H, t, *J* = 5.94 Hz)
H-3′	7.18 (1 H, d, *J* = 15.60 Hz)	7.23 (1 H, d, *J* = 15.66 Hz)	7.20 (1 H, d, *J* = 15.60 Hz)	7.23 (1 H, d, *J* = 15.66 Hz)	7.21 (1 H, d, *J* = 15.60 Hz)	7.22 (1 H, d, *J* = 15.60 Hz)	7.30 (1 H, d, *J* = 15.66 Hz)
H-2″	7.06 (1 H, d, *J* = 1.92 Hz	6.94 (1 H, d *J* = 2.04 Hz)	6.94 (1 H, s)	6.94 (1 H, d, *J* = 1.95 Hz)	6.94 (1 H, d, *J* = 2.04 Hz)	6.93 (1 H, d, *J* = 1.86 Hz)	6.99 (1 H, d, *J* = 1.92 Hz)
H-6″	6.80 (1 H, dd, *J* = 8.10, 1.92 Hz)	6.83 (1 H, dd, *J* = 8.10, 2.04 Hz)	6.69 (1 H, d, *J* = 7.92 Hz)	6.83 (1 H, dd, *J* = 8.10, 1.95 Hz)	6.84 (1 H, dd, *J* = 8.10, 2.04 Hz)	6.83 (1 H, dd, *J* = 8.10, 1.86 Hz)	6.85 (1 H, dd, *J* = 8.22, 2.04 H)
H-5″	6.72 (1 H, d, *J* = 8.10, Hz)	6.74 (1 H, d, *J* = 8.10 Hz)	6.77 (1 H, d, *J* = 7.92 Hz)	6.74 (1 H, d, *J* = 8.10 Hz)	6.73 (1 H, d, *J* = 8.10 H)	6.74 (1 H, d, *J* = 8.10 H)	6.76 (1 H, d, *J* = 8.22 Hz)
H-2′	6.55 (1 H, d, *J* = 15.60 Hz)	6.34 (1 H, d, *J* = 15.66 Hz)	6.30 (1 H, d, *J* = 15.60 Hz)	6.32 (1 H, d, *J* = 15.66 Hz)	6.28 (1 H, d, *J* = 15.60 Hz)	6.35 (1 H, d, *J* = 15.60 Hz)	6.43 (1 H, d, *J* = 15.66 Hz)
H-1	N/A	N/A	N/A	N/A	2.60 (2 H, t, *J* = 7.32 Hz)	2.14–2.10 (1 H, m)	N/A
H-2	3.55 (2 H, d, *J* = 4.80 Hz)	2.43 (2 H, t, *J* = 6.75 Hz)	2.04 (2 H, t, *J* = 6.78)	2.20 (2 H, t, *J* = 7.30 Hz)	3.42 (2 H, m)	1.90–1.73 (4 H, m)	7.89 (2 H, d, *J* = 8.22 Hz)
H-3	N/A	3.35 (2 H, m)	1.65 (2 H, m)	1.52–1.39 (4 H, m)	N/A	1.29–0.89 (4 H, m)	7.34 (2 H, d, *J* = 8.22 Hz)
H-4	N/A	N/A	3.13 (2 H, s)	1.32–1.25 (2 H, m)	N/A	1.43–1.33 (1 H, m)	N/A
H-5	N/A	N/A	N/A	1.52–1.39 (4 H, m)	N/A	1.29–0.89 (4 H, m)	7.34 (2 H, d, *J* = 8.22 Hz)
H-6	N/A	N/A	N/A	3.14 (2 H, m)	N/A	1.90–1.73 (4 H, m)	7.89 (2 H, d, *J* = 8.22 Hz)
–CH_2–	N/A	N/A	N/A	N/A	N/A	3.01 (2 H, t, *J* = 5.82 Hz	4.43 (2 H, d, *J* = 5.94 Hz)

1.2 p-Hydroxycinnamic acid derivatives

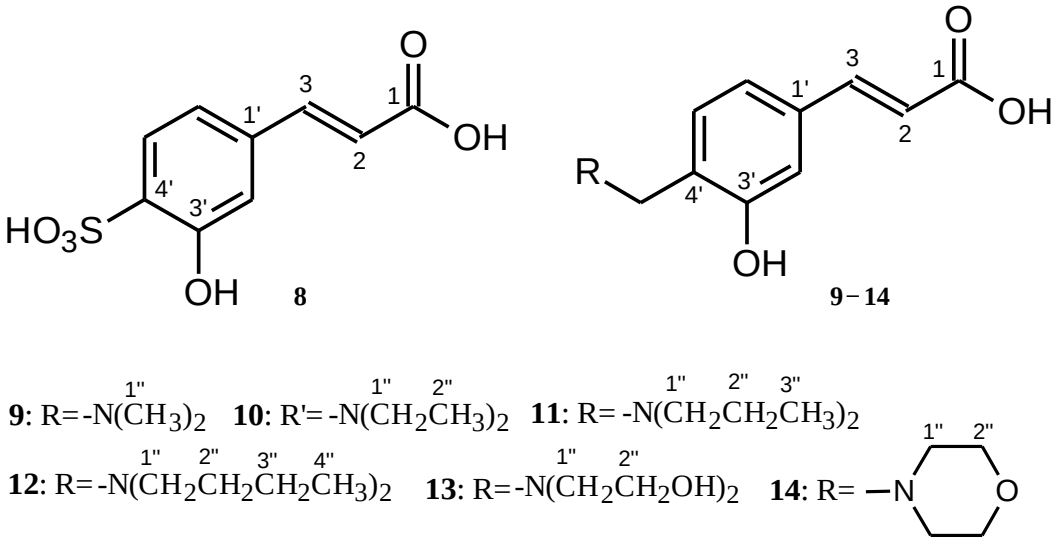


Figure S2 The Structures of Cds. **8**–**14**

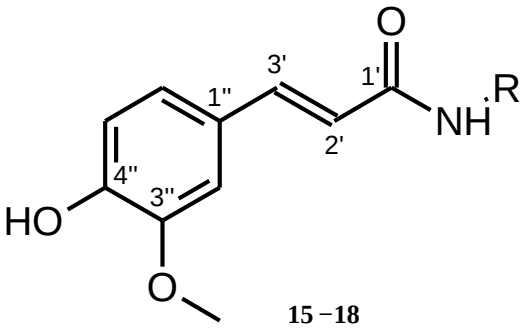
Table S3 ^{13}C NMR Data of Cds. **8**–**14** (151 MHz, DMSO-d_6)

	Cd. **8**	Cd. **9**	Cd. **10**	Cd. **11**	Cd.**12**	Cd. **13**	Cd. **14**
–CH_2–	N/A	57.71	54.95	53.55	51.66	54.94	53.41
C-1	167.55	172.19	167.84	167.28	167.31	172.10	167.33
C-2	118.49	119.76	118.95	119.53	119.05	119.80	118.98
C-3	143.22	146.52	143.59	143.29	143.27	146.45	143.31
C-1′	136.82	138.59	134.40	136.63	136.62	138.59	136.83
C-2′	116.11	115.97	114.45	114.73	114.76	115.79	114.84
C-3′	153.57	157.40	157.97	156.99	157.02	157.19	157.16
C-4′	132.17	119.72	125.15	118.68	118.60	119.50	117.57
C-5′	127.67	133.86	129.21	133.47	133.53	133.71	133.98
C-6′	120.27	121.41	119.17	120.12	120.08	121.64	120.14
C-1″	N/A	43.49	45.90	50.49	50.20	56.21	63.05
C-2″	N/A	N/A	10.98	16.53	24.82	55.95	50.72
C-3″	N/A	N/A	N/A	11.00	19.53	N/A	N/A
C-4″	N/A	N/A	N/A	N/A	13.53	N/A	N/A

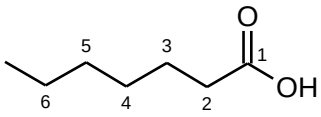
Table S4 ^{1}H NMR Data of Cds. **8**–**14** (600 MHz, DMSO-d_6)

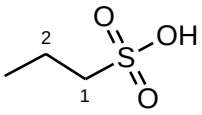
	Cd. **8**	Cd. **9**	Cd. **10**	Cd. **11**	Cd.**12**	Cd. **13**	Cd. **14**
−COOH	N/A	N/A	N/A	10.65 (1 H, s)	12.49 (1 H, s)	11.29 (1 H, s)	12.50 (1 H, s)
−OH	10.52 (1 H, s)	N/A	N/A	10.01 (1 H, s)	10.18 (1 H, s)	N/A	10.64 (1 H, s)
R_3NH^+	N/A	N/A	N/A	N/A	10.71 (1 H, s)	N/A	11.05 (1 H, s)
$-CH_2-$	N/A	4.37 (2 H, s)	3.75 (2 H, s)	4.21 (2 H, s)	4.22 (2 H, s)	4.59 (2 H, s)	4.25 (2 H, s)
H-2	6.48 (2 H, d, *J* = 16.02 Hz)	6.52 (1 H, d, *J* = 15.96 Hz)	6.97 (1 H, s)	6.44 (1 H, d, *J* = 15.96 Hz)	6.44 (1 H, d, *J* = 15.96 Hz)	6.53 (1 H, d, *J* = 15.96 Hz)	6.44 (1 H, d, *J* = 15.96 Hz)
H-3	7.49 (1 H, d, *J* = 16.02 Hz)	7.70 (1 H, d, *J* = 15.96 Hz)	7.46 (1 H, d, *J* = 15.96 Hz)	7.49 (1 H, d, *J* = 15.96 Hz)	7.49 (1 H, d, *J* = 15.96 Hz)	7.70 (1 H, d, *J* = 15.96 Hz)	7.50 (1H, d, *J* = 15.96 Hz)
H-2′	7.09 (1 H, d, *J* = 1.68 Hz)	7.25 (1 H, d, *J* = 1.08 Hz)	6.42 (1 H, d, *J* = 15.96 Hz)	7.24 (1 H, s)	7.26 (1 H, s)	7.26 (1 H, s)	7.24 (1 H, d, *J* = 1.26 Hz)
H-5′	7.46 (1 H, d, *J* = 7.86 Hz)	7.40 (1 H, d, *J* = 7.80, 1.08 Hz)	7.03 (1 H, d, *J* = 7.80 Hz)	7.19 (1 H, d, *J* = 7.86 Hz)	7.58 (1 H, d, *J* = 7.92 Hz)	7.18 (1 H, d, *J* = 7.86 Hz)	7.58 (1 H, d, *J* = 7.86 Hz)
H-6′	7.13 (1 H, dd, *J* = 7.86, 1.68 Hz)	7.18 (1 H, d, *J* = 7.80 Hz)	7.10 (1 H, d, *J* = 7.80 Hz)	7.54 (1 H, d, *J* = 7.86 Hz)	7.19 (1 H, d, *J* = 7.92 Hz)	7.40 (1 H, d, *J* = 7.86 Hz)	7.20 (1 H, dd, *J* = 7.86, 1.26 Hz)
H-1″	N/A	2.93 (6 H, s)	2.56 (4 H, m)	2.93 (4 H, t, *J* = 8.04 Hz)	2.96 (4 H, t)	3.50 (4 H, t, *J* = 4.92 Hz)	3.86 (4 H, m)
H-2″	N/A	N/A	1.02 (6 H, t, *J* = 7.14 Hz)	1.73 (4H, m, H-2″)	1.73–1.68 (4 H, m)	4.05 (4 H, t, *J* = 4.92 Hz	3.16 (4 H, m)
H-3″	N/A	N/A	N/A	0.86 (6H, t, *J* = 7.32 Hz)	1.28–1.25 (4 H, m)	N/A	N/A
H-4″	N/A	N/A	N/A	N/A	0.88–0.85 (6H, t, *J* = 7.38 Hz)	N/A	N/A

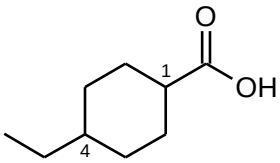
1.3 Ferulic acid derivatives



15 −18

15: R= 

16: R= 

17: R= 

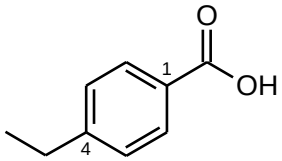
18: R= 

Figure S3 The Structures of Cds. **15–18**

Table S5 ^{13}C NMR Data of Cds. **15–18** (151 MHz, DMSO-d_6)

	Cd. **15**	Cd. **16**	Cd. **17**	Cd. **18**
−COOH	N/A	N/A	176.77	167.23
−OCH_3	55.98	58.54	55.51	55.55
CH_2−	N/A	N/A	42.52	42.07
C-1	174.49	52.66	44.75	126.35
C-2	34.09	38.15	29.51	129.44
C-3	24.72	N/A	28.31	127.27
C-4	26.51	N/A	37.17	N/A
C-5	29.42	N/A	28.31	127.27
C-6	39.96	N/A	29.51	129.44
C-1′	165.73	171.60	165.39	165.61
C-2′	119.56	119.96	119.12	118.59
C-3′	139.24	144.03	138.83	139.63
C-1″	126.93	130.04	126.50	129.36
C-2″	111.16	113.80	110.65	110.87
C-3″	148.65	150.21	148.20	148.39
C-4″	148.27	149.77	147.82	144.82
C-5″	116.10	118.21	115.65	115.69
C-6″	121.95	125.35	121.51	121.66

Table S6 ^{1}H NMR Data of Cds. **15**–**18** (600 MHz, DMSO-d_6)

	Cd. **15**	Cd. **16**	Cd. **17**	Cd. **18**
−COOH	12.00 (1 H, s)	N/A	12.00 (1 H, s)	12.85 (1 H, s)
−OH	9.41 (1 H, s)	N/A	9.40 (1 H, s)	9.46 (1 H, s)
−CONH−	7.93 (1 H, t, *J* = 5.49 Hz)	N/A	7.93 (1 H, t, *J* = 6.27 Hz)	8.56 (1 H, t, *J* = 6.00 Hz)
−OCH_3	3.80 (3 H, s)	3.79 (3 H, s)	3.80 (3 H, s)	3.80 (3 H, s)
−CH_2−	N/A		3.02 (2 H, t, *J* = 6.27 Hz)	4.46 (2 H, d, *J* = 6.00 Hz)
H-1	N/A	3.64 (2 H, t, *J* = 6.93 Hz)	2.15–2.09 (1 H, m)	N/A
H-2	2.20 (2 H, t, *J* = 7.38 Hz)	3.14 (2 H, t, *J* = 6.93 Hz)	1.91–1.74 (2 H, m)	7.91 (1 H, d, *J* = 8.28 Hz)
H-3	1.53–1.41 (2 H, m)	N/A	1.29–0.90 (2 H, m)	7.40 (1 H, d, *J* = 8.28 Hz)
H-4	1.31–1.26 (2 H, m)	N/A	1.41–1.35 (1 H, m)	N/A
H-5	1.53–1.41 (2 H, m)	N/A	1.29–0.90 (2 H, m)	7.40 (1 H, d, *J* = 8.28 Hz)
H-6	3.14 (2 H, m)	N/A	1.91–1.74 (2 H, m)	7.91 (1 H, d, *J* = 8.28 Hz)
H-2′	6.43 (1 H, d, *J* = 15.66 Hz)	6.21 (1 H, d, *J* = 15.78 Hz)	6.47 (1 H, d, *J* = 15.72 Hz)	6.53 (1 H, d, *J* = 15.72 Hz)
H-3′	7.30 (1 H, d, *J* = 15.66 Hz)	7.21 (1 H, d, *J* = 15.78 Hz)	7.31 (1 H, d, *J* = 15.72 Hz)	7.38 (1 H, d, *J* = 15.72 Hz)
H-2″	7.11 (1 H, s)	6.95 (1 H, t, *J* = 1.74 Hz)	7.11 (1 H, d, *J* = 1.74 Hz)	7.15 (1 H, d, *J* = 1.86 Hz)
H-5″	6.98 (1 H, d, *J* = 8.10 Hz)	6.79 (1 H, t, *J* = 8.04 Hz)	6.78 (1 H, d, *J* = 8.10 Hz)	6.80 (1 H, d, *J* = 8.16 Hz)
H-6″	6.78 (1 H, d, *J* = 8.10 Hz)	6.94 (1 H, dd, *J* = 8.04, 1.74 Hz)	6.98 (1 H, dd, *J* = 8.10, 1.74 Hz)	7.01 (1 H, dd, *J* = 8.16, 1.86 Hz)

2. Molecule Structures of Compounds 4, 6, and 7

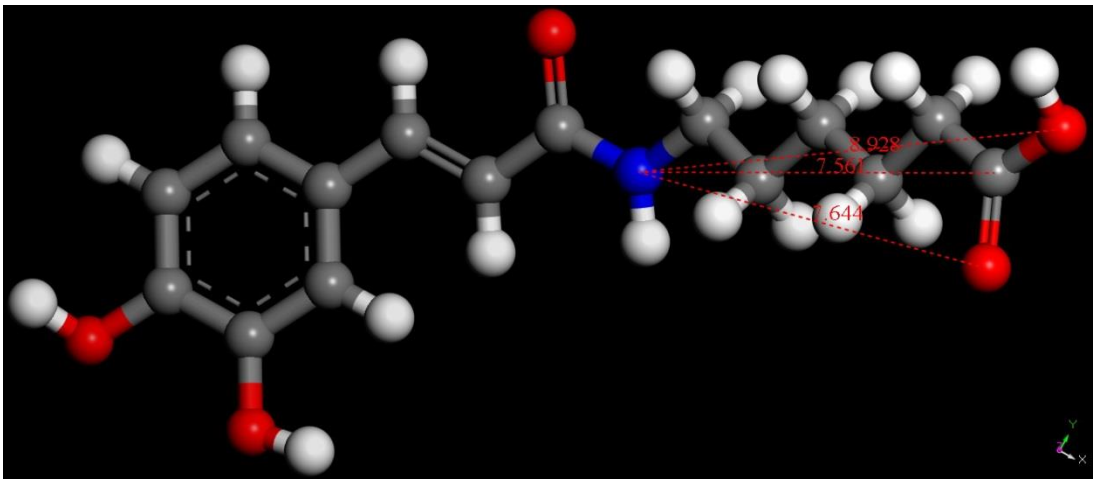


Figure 1 Molecule Structures of Cd. 4

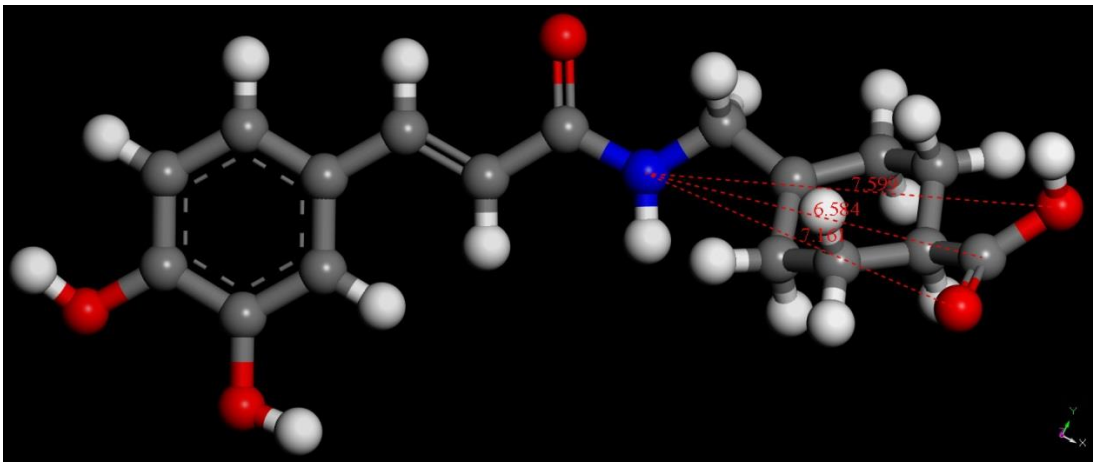


Figure 2 Molecule Structures of Cd. 6

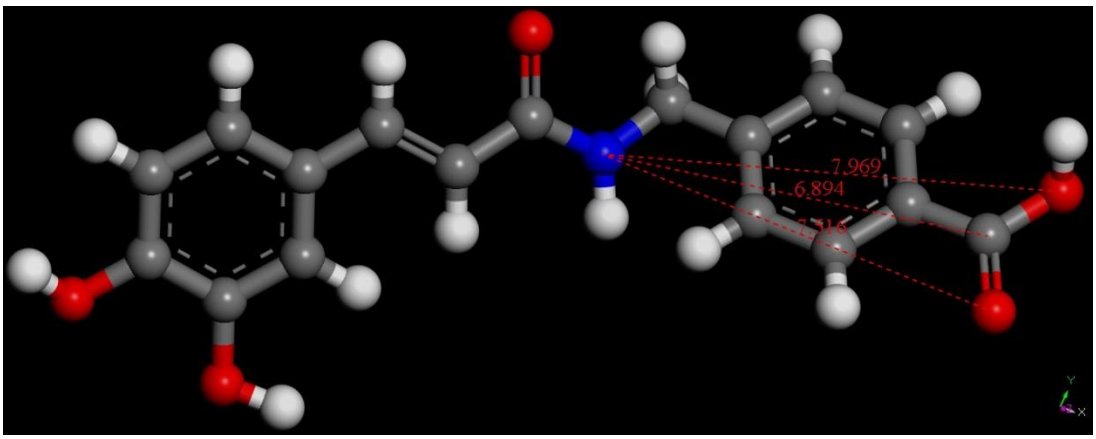


Figure 3 Molecule Structures of Cd. 7